

2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine
368441-96-7 | DTXSID50364048

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.84e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.44e-01

Confidence level: 4.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Nabam-sodium</div> <div>Measured: 7.80e-01</div> <div>Predicted: 2.66e-01</div>	<div>Image not found</div> <div>Sparteine</div> <div>Measured: 1.30e-02</div> <div>Predicted: 8.29e-03</div>	<div>Image not found</div> <div>Bis(ethylxanthogen)</div> <div>Measured: 1.14e-05</div> <div>Predicted: 4.06e-05</div>
<div>Image not found</div> <div>Heptachlor epoxide</div> <div>Measured: 5.14e-07</div> <div>Predicted: 3.52e-07</div>		